

Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.95	17.73
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.69	-1.38

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:47:26 ON 27 APR 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1204jxv

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 15:38:05 ON 27 APR 2004
FILE 'CAPLUS' ENTERED AT 15:38:05 ON 27 APR 2004
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.95	17.73
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.69	-1.38

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.38	18.16
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.69	-1.38

FILE 'REGISTRY' ENTERED AT 15:38:45 ON 27 APR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 25 APR 2004 HIGHEST RN 676591-92-7
DICTIONARY FILE UPDATES: 25 APR 2004 HIGHEST RN 676591-92-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

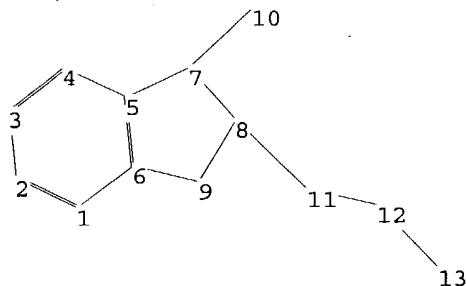
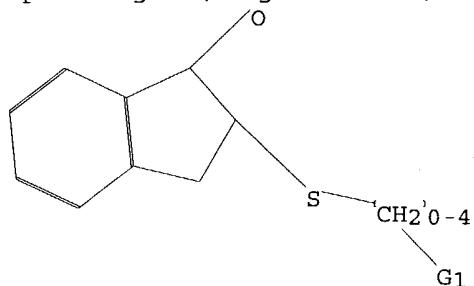
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10692735.str



chain nodes :

10 11 12 13

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

7-10 8-11 11-12 12-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

5-7 6-9 7-8 7-10 8-9 8-11 12-13

exact bonds :

11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:Cy,Ak

Connectivity :

11:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

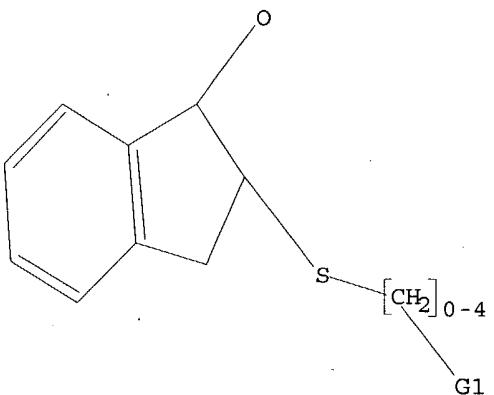
11:CLASS 12:CLASS 13:CLASS

L5 STRUCTURE UPLOADED

=> d

L5 HAS NO ANSWERS

L5 STR



G1 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 15:39:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1792 TO ITERATE

55.8% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

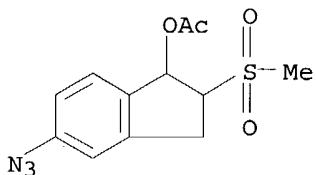
3 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 33301 TO 38379
PROJECTED ANSWERS: 3 TO 246

L6 3 SEA SSS SAM L5

=> d scan

L6 3 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 5-azido-2,3-dihydro-2-(methylsulfonyl)-, acetate (ester)
(9CI)
MF C12 H13 N3 O4 S

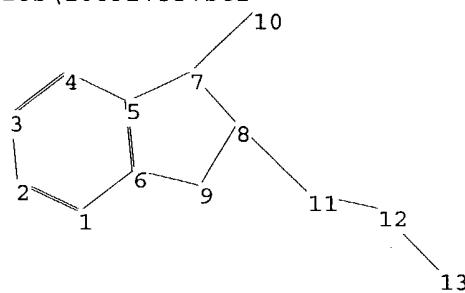
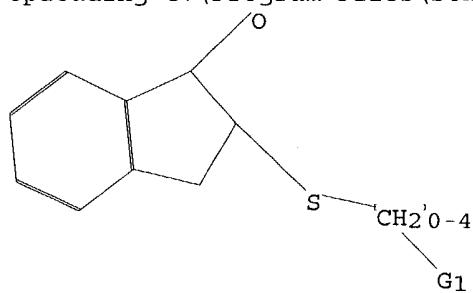


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>
Uploading C:\Program Files\Stnexp\Queries\10692735.str



chain nodes :
10 11 12 13
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
7-10 8-11 11-12 12-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 7-10 8-9 8-11 12-13
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:Cy,Ak

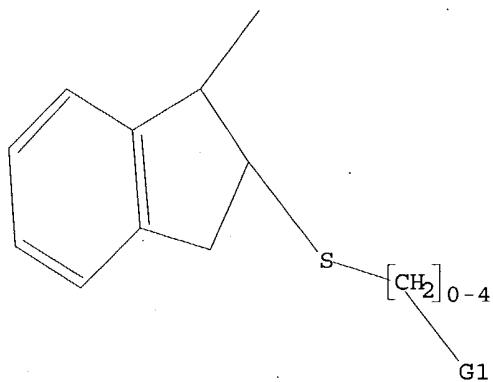
Connectivity :
11:2 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS

L7 STRUCTURE UPLOADED

=> que L7

L8 QUE L7

=> d
L8 HAS NO ANSWERS
L7 STR



G1 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.
L8 QUE ABB=ON PLU=ON L7

=> s 17
SAMPLE SEARCH INITIATED 15:39:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1792 TO ITERATE

55.8% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

1 ANSWERS

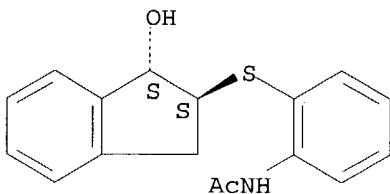
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTION ITERATIONS: 33301 TO 38379
PROJECTION ANSWERS: 1 TO 115

L9 1 SEA SSS SAM L7

=> d scan

L9 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetamide, N-[2-[(2,3-dihydro-1-hydroxy-1H-inden-2-yl)thio]phenyl]-, trans- (9CI)
MF C17 H17 N O2 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s 17 full
FULL SEARCH INITIATED 15:40:15 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 35757 TO ITERATE

100.0% PROCESSED 35757 ITERATIONS
SEARCH TIME: 00.00.01

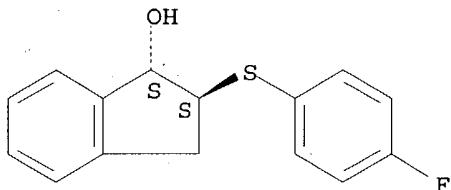
71 ANSWERS

L10 71 SEA SSS FUL L7

=> d scan

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2-[(4-fluorophenyl)thio]-2,3-dihydro-, trans- (9CI)
MF C15 H13 F O S

Relative stereochemistry.

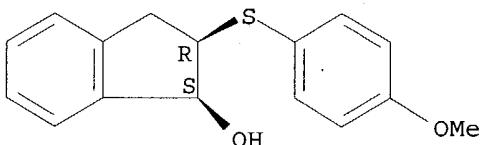


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 2,3-dihydro-2-[(4-methoxyphenyl)thio]-, cis- (9CI)
MF C16 H16 O2 S

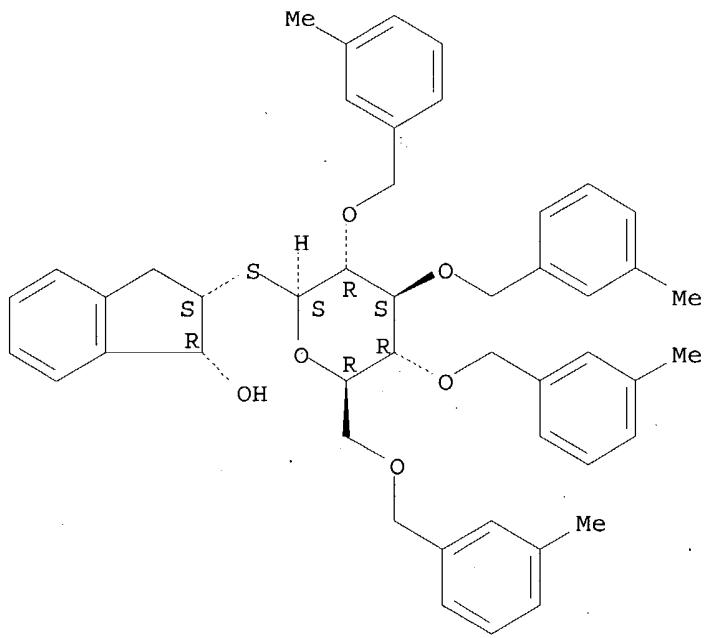
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

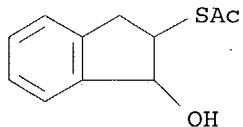
L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN β -D-Glucopyranoside, (1R,2S)-2,3-dihydro-1-hydroxy-1H-inden-2-yl
2,3,4,6-tetrakis-O-[(3-methylphenyl)methyl]-1-thio- (9CI)
MF C47 H52 O6 S

Absolute stereochemistry.



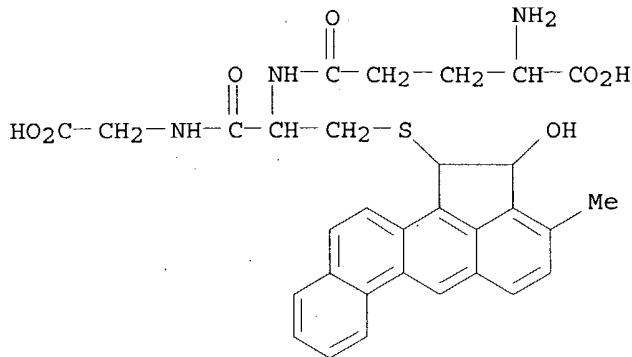
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Acetic acid, thio-, S-1-hydroxy-2-indanyl ester (7CI)
 MF C11 H12 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

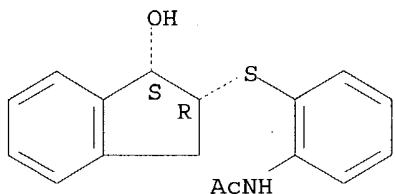
L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Glycine, N-[S-(1,2-dihydro-2-hydroxy-3-methylbenz[j]aceanthrylen-1-yl)-N-L- γ -glutamyl-L-cysteinyl]- (9CI)
 MF C31 H31 N3 O7 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Acetamide, N-[2-[(2,3-dihydro-1-hydroxy-1H-inden-2-yl)thiophenyl]-, cis-
 (9CI)
 MF C17 H17 N O2 S

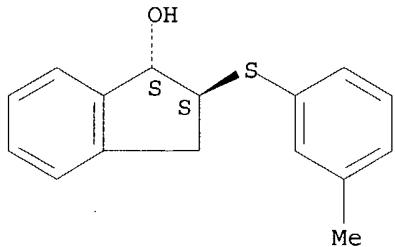
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 1H-Inden-1-ol, 2,3-dihydro-2-[(3-methylphenyl)thio]-, trans- (9CI)
 MF C16 H16 O S

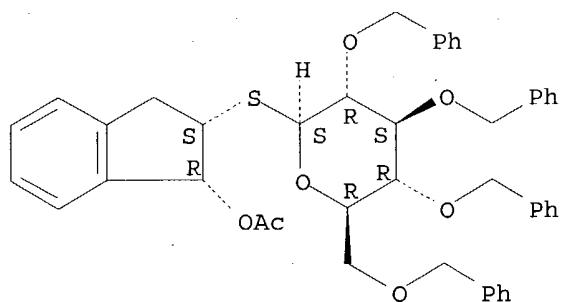
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

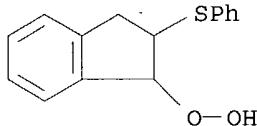
L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN β -D-Glucopyranoside, (1R,2S)-1-(acetyloxy)-2,3-dihydro-1H-inden-2-yl
2,3,4,6-tetrakis-O-(phenylmethyl)-1-thio- (9CI)
MF C45 H46 O7 S

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

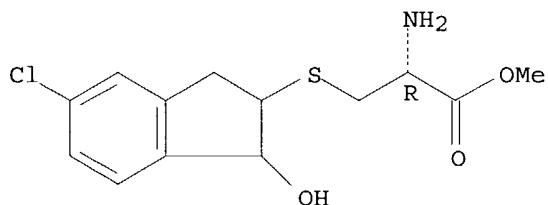
L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Hydroperoxide, 2-(phenylthio)-1-indanyl (6CI, 7CI)
MF C15 H14 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN L-Cysteine, S-(5-chloro-2,3-dihydro-1-hydroxy-1H-inden-2-yl)-, methyl
ester (9CI)
MF C13 H16 Cl N O3 S

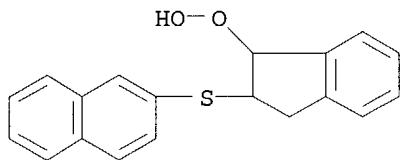
Absolute stereochemistry.



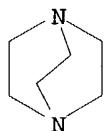
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS . REGISTRY COPYRIGHT 2004 ACS on STN
IN Hydroperoxide, 2-(2-naphthylthio)-1-indanyl, compd. with
1,4-diazabicyclo[2.2.2]octane (7CI)
MF C19 H16 O2 S . 1/2 C6 H12 N2

CM 1



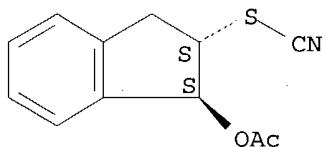
CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L10. 71 ANSWERS . REGISTRY COPYRIGHT 2004 ACS on STN
IN Thiocyanic acid, 1-(acetyloxy)-2,3-dihydro-1H-inden-2-yl ester, trans-
(9CI)
MF C12 H11 N O2 S

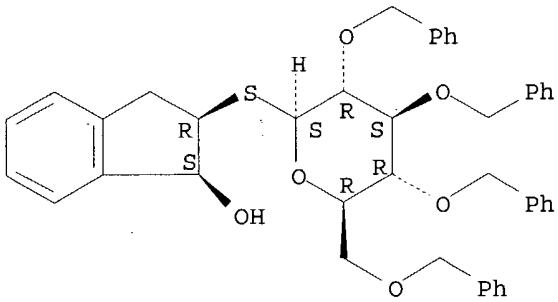
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS . REGISTRY COPYRIGHT 2004 ACS on STN
IN β -D-Glucopyranoside, (1S,2R)-2,3-dihydro-1-hydroxy-1H-inden-2-yl
2,3,4,6-tetrakis-O-(phenylmethyl)-1-thio- (9CI)
MF C43 H44 O6 S

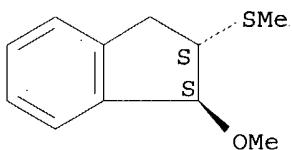
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

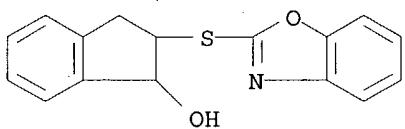
L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 1H-Indene, 2,3-dihydro-1-methoxy-2-(methylthio)-, trans- (9CI)
 MF C11 H14 O S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

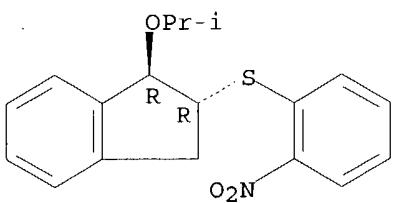
L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 1H-Inden-1-ol, 2-(2-benzoxazolylthio)-2,3-dihydro- (9CI)
 MF C16 H13 N O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 1H-Indene, 2,3-dihydro-1-(1-methylethoxy)-2-[(2-nitrophenyl)thio]-, trans- (9CI)
 MF C18 H19 N O3 S

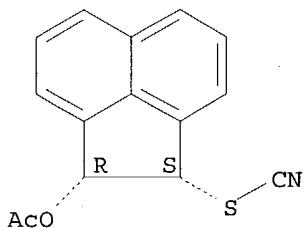
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN Thiocyanic acid, 2-(acetyloxy)-1,2-dihydro-1-acenaphthylenyl ester, cis-
 (9CI)
 MF C15 H11 N O2 S

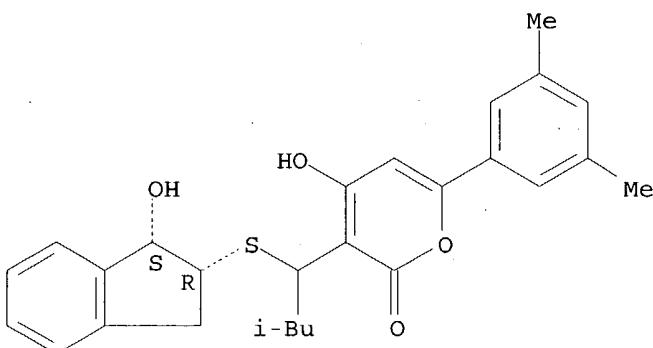
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 2H-Pyran-2-one, 3-[1-[(1R,2S)-2,3-dihydro-1-hydroxy-1H-inden-2-yl]thio]-3-
 methylbutyl]-6-(3,5-dimethylphenyl)-4-hydroxy-, rel- (9CI)
 MF C27 H30 O4 S

Relative stereochemistry.

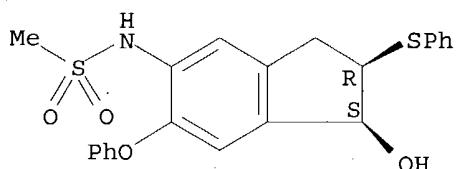


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

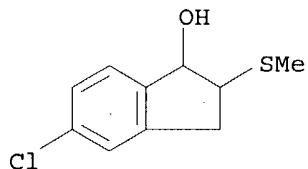
IN Methanesulfonamide, N-[2,3-dihydro-1-hydroxy-6-phenoxy-2-(phenylthio)-1H-inden-5-yl]-, cis- (9CI)
MF C22 H21 N O4 S2

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

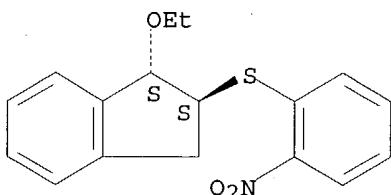
L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylthio)- (9CI)
MF C10 H11 Cl O S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 71 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Indene, 1-ethoxy-2,3-dihydro-2-[(2-nitrophenyl)thio]-, trans- (9CI)
MF C17 H17 N O3 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
156.26	174.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.38

FILE 'CAPLUS' ENTERED AT 15:40:45 ON 27 APR 2004
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FILE COVERS 1907 - 27 Apr 2004 VOL 140 ISS 18
 FILE LAST UPDATED: 26 Apr 2004 (20040426/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l10
 L11 38 L10

=> s l11 and pharmaceut?
 246583 PHARMACEUT?
 L12 3 L11 AND PHARMACEUT?

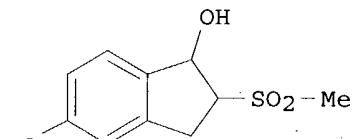
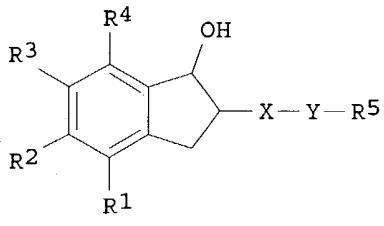
=> d ibib abs hitstr 1-3

L12 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2003:202618 CAPLUS
 DOCUMENT NUMBER: 138:221365
 TITLE: Preparation of indan-1-ols as appetite depressants
 INVENTOR(S): Jaehne, Gerhard; Krone, Volker; Bickel, Martin;
 Gossel, Matthias
 PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
 SOURCE: PCT Int. Appl., 53 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020696	A1	20030313	WO 2002-EP9206	20020817
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10142667	A1	20030327	DE 2001-10142667	20010831

US 2003114681	A1 20030619	US 2002-231394	20020830
US 6657086	B2 20031202		
US 2004068016	A1 20040408	US 2003-665021	20030922
PRIORITY APPLN. INFO.:		DE 2001-10142667 A	20010831
		US 2002-231394	A3 20020830

OTHER SOURCE(S) : MARPAT 138:221365
GI



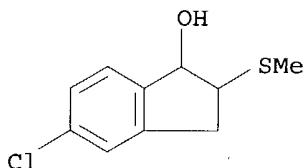
AB Title compds. I [R1, R2, R3, R4 = H, halo, CN, etc.; X = S, SO, SO₂; Y = (CH₂)_p; p = 0-3; R5 = CF₃, alkyl, cycloalkyl] and their pharmaceutically acceptable salts were prepared. For example, NaBH₄ mediated reduction of 5-chloro-2-methylsulfonylindan-1-one, e.g., prepared from 2-bromo-5-chloroindan-1-one in 2-steps, provided indanol II. In milk consumption studies with female NMRI mice, indanol II exhibited very good anorectic effects, i.e., 50% decrease in milk consumption versus control.

IT 500910-95-2P 500910-98-5P 500911-00-2P
500911-04-6P 500911-05-7P 500911-08-0P
500911-10-4P 500911-11-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of indanols as appetite depressants)

RN 500910-95-2 CAPLUS

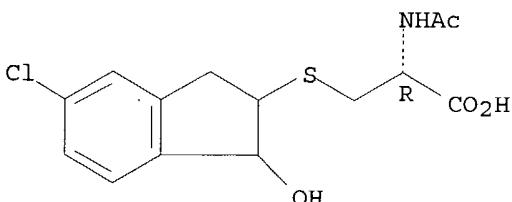
CN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(methylthio)- (9CI) (CA INDEX NAME)



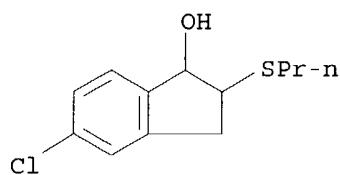
RN 500910-98-5 CAPLUS

CN L-Cysteine, N-acetyl-S-(5-chloro-2,3-dihydro-1-hydroxy-1H-inden-2-yl)- (9CI) (CA INDEX NAME)

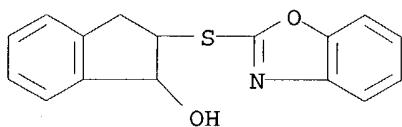
Absolute stereochemistry.



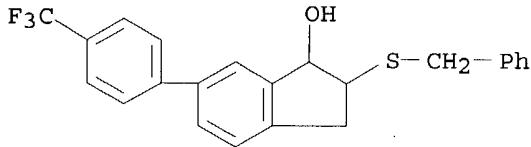
RN 500911-00-2 CAPLUS
CN 1H-Inden-1-ol, 5-chloro-2,3-dihydro-2-(propylthio)- (9CI) (CA INDEX NAME)



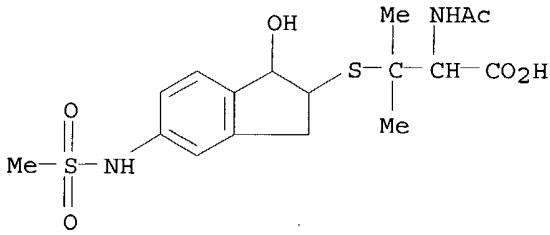
RN 500911-04-6 CAPLUS
CN 1H-Inden-1-ol, 2-(2-benzoxazolylthio)-2,3-dihydro- (9CI) (CA INDEX NAME)



RN 500911-05-7 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-2-[(phenylmethyl)thio]-6-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

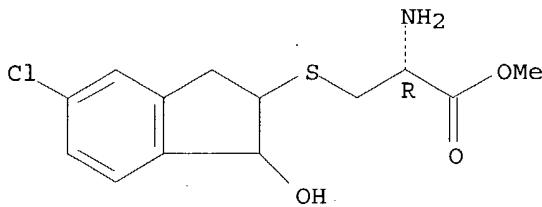


RN 500911-08-0 CAPLUS
CN Valine, N-acetyl-3-[[2,3-dihydro-1-hydroxy-5-[(methylsulfonyl)amino]-1H-inden-2-yl]thio]- (9CI) (CA INDEX NAME)

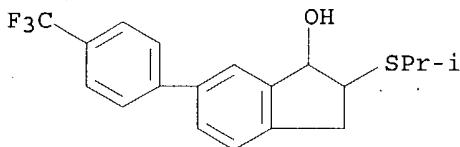


RN 500911-10-4 CAPLUS
CN L-Cysteine, S-(5-chloro-2,3-dihydro-1-hydroxy-1H-inden-2-yl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



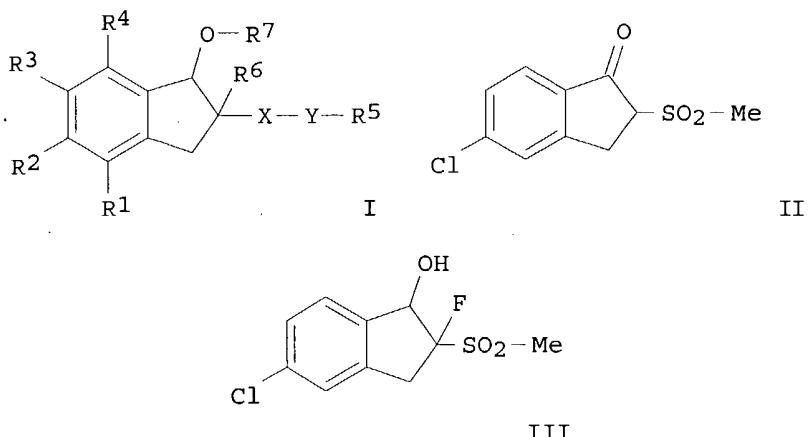
RN 500911-11-5 CAPLUS
 CN 1H-Inden-1-ol, 2,3-dihydro-2-[(1-methylethyl)thio]-6-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2003:202617 CAPLUS
 DOCUMENT NUMBER: 138:221364
 TITLE: Preparation of 2-fluoro-1-indanols and their use as appetite depressants
 INVENTOR(S): Jaehne, Gerhard; Krone, Volker; Bickel, Martin;
 Gossel, Matthias
 PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
 SOURCE: PCT Int. Appl., 49 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020695	A1	20030313	WO 2002-EP9203	20020817
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10142663	A1	20030327	DE 2001-10142663	20010831
US 2003181491	A1	20030925	US 2002-231418	20020829
PRIORITY APPLN. INFO.:			DE 2001-10142663 A	20010831
OTHER SOURCE(S):		MARPAT 138:221364		
GI				



AB Title compds. I [R1, R2, R3, R4 = H, halo, CN, etc.; X = S, SO, SO₂; Y = (CH₂)_p; p = 0-3; R5 = CF₃, alkyl, cycloalkyl; R9 = substituted alkyl or cycloalkyl, e.g. F, CO, CO₂, etc.] and their **pharmaceutically** acceptable salts were prepared. For example, fluorination of indanone II, e.g., prepared from 2-bromo-5-chloroindan-1-one in 2-steps, followed by NaBH₄ mediated reduction provided fluoroindanol III. In milk consumption studies with female NMRI mice, indanol III exhibited very good anorectic effects, i.e., 46% reduction of milk consumption verses control.

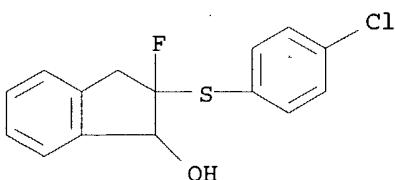
IT 500899-40-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of fluoroindanols as appetite depressants)

RN 500899-40-1 CAPLUS

CN 1H-Inden-1-ol, 2-[(4-chlorophenyl)thio]-2-fluoro-2,3-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:639087 CAPLUS

DOCUMENT NUMBER: 93:239087

TITLE: Indanyl derivatives and **pharmaceutical** preparations containing them

INVENTOR(S): Schroeder, Eberhard; Rufer, Clemens; Boettcher, Irmgard

PATENT ASSIGNEE(S): Schering A.-G., Fed. Rep. Ger.

SOURCE: Brit. UK Pat. Appl., 19 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent

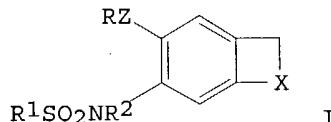
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2025973	A	19800130	GB 1979-26016	19790726
DE 2833202	A1	19800214	DE 1978-2833202	19780727
DE 2923937	A1	19810108	DE 1979-2923937	19790611
DD 145101	C	19801119	DD 1979-214579	19790724
PL 126816	B1	19830930	PL 1979-217384	19790725
FI 7902347	A	19800128	FI 1979-2347	19790726
FI 71306	B	19860909		
FI 71306	C	19861219		
DK 7903159	A	19800128	DK 1979-3159	19790726
DK 159269	B	19900924		
DK 159269	C	19910218		
NO 7902474	A	19800129	NO 1979-2474	19790726
NO 147560	B	19830124		
NO 147560	C	19830504		
FR 2433512	A1	19800314	FR 1979-19301	19790726
SU 965352	A3	19821007	SU 1979-2789351	19790726
IL 57901	A1	19831130	IL 1979-57901	19790726
HU 29615	O	19840228	HU 1979-SE684	19790726
HU 184679	B	19840928		
AU 7949325	A1	19800207	AU 1979-49325	19790727
AU 532405	B2	19830929		
JP 55020777	A2	19800214	JP 1979-95152	19790727
JP 63010696	B4	19880308		
ES 482918	A1	19800516	ES 1979-482918	19790727
ZA 7903854	A	19800730	ZA 1979-3854	19790727
US 4244960	A	19810113	US 1979-61779	19790727
RO 78632	P	19820412	RO 1979-98285	19790727
CA 1124724	A1	19820601	CA 1979-332665	19790727
CS 242855	B2	19860515	CS 1979-5235	19790727
PRIORITY APPLN. INFO.:			DE 1978-2833202	19780727
			DE 1979-2923937	19790611

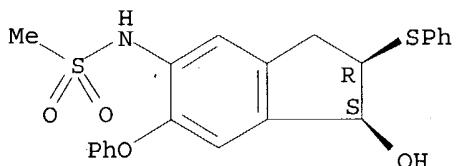
GI



AB Title compds. I [R = Ph or pyridyl optionally substituted by ≥ 1 halo, C1-4 alkyl, CF₃; Z = O, S; R1 = C1-4 alkyl optionally substituted by ≥ 1 F or Cl; R2 = R1SO₂ (R1 same as above), C1-6 acyl, H; X = (CH₂)₂, CH:CH, C(Z₁)CH₂ (Z₁ = O, NOH, C1-4 alkoxyimino, phenylhydrazone, p-toluenesulfonylhydrazone), CHR₃CH₂ [R₃ = OH, C1-6 acyloxy, R₁SO₂NH, R₁SO₃ (R1 same as above), NH₂, C1-6 acylamino, cyano], CHR₃CH(SO_nR₄) or C(Z₁)CH(SO_nR₄) (n = 0, 1, 2; R₄ = C1-4 alkyl, Ph optionally substituted by halo, C1-4 alkyl, NO₂, CO₂H; Z₁, R₃ same as above)] were prepared and showed antiinflammatory activity. Thus, N-(6-phenoxy-5-indanyl)methanesulfonamide was prepared from 5-bromo-6-nitroindan by sequential reaction with PhOH (CuCl-K₂CO₃, refluxing pyridine, 3 h), reduction (H/Raney Ni), and treatment with MeSO₂Cl in pyridine at 0° and room temperature. I showed superior activity to indomethacin, especially dissociation between antiinflammatory and ulcerogenic activity. I barely inhibits the synthesis of prostaglandin. I also show herbicidal activity (no data). IT 75361-01-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 75361-01-2 CAPLUS
CN Methanesulfonamide, N-[2,3-dihydro-1-hydroxy-6-phenoxy-2-(phenylthio)-1H-inden-5-yl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



=> s C17 H17 N O2 S/mf and 111

REGISTRY INITIATED

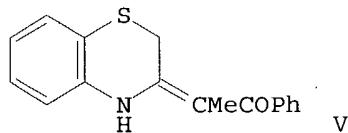
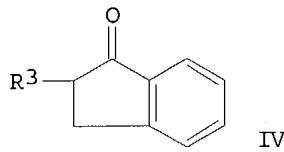
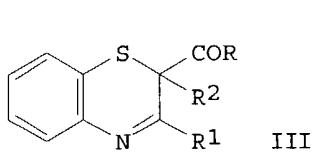
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L14 651 L13

L15 1 L14 AND L11

=> d ibib abs hitstr

L15 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:35781 CAPLUS
DOCUMENT NUMBER: 112:35781
TITLE: Reaction of 2,2'-dithiodianiline with
2-alkyl-1,3-diketones. Synthesis and chemical
behavior of some 2-acyl-2H-1,4-benzothiazines
AUTHOR(S): Trapani, Giuseppe; Latrofa, Andrea; Reho, Antonia;
Liso, Gaetano
CORPORATE SOURCE: Dip. Farm.-Chim., Univ. Bari, Bari, 70126, Italy
SOURCE: Journal of Heterocyclic Chemistry (1989), 26(3), 721-4
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:35781
GI



AB The reaction of 2-H2NC6H4SSC6H4NH2-2 (I) with 2-alkyl-1,3-diketones to synthesize 2-acyl-2H-1,4-benzothiazines was studied. In the cases of I with RCOCHR2COR1 (II, RR1 = o-C6H4CH2CH2, R2 = Me; R = R1 = Ph, R2 = Me), the expected 2-acyl-2H-1,4-benzothiazines, i.e. III, were obtained, whereas the reactions of I with the 1,3-diketones IV (R3 = COMe) and II (R = Ph, R1 = R2 = Me) afforded the α -ketosulfide IV (R3 = 2-AcNHC6H4S) and the 1,4-benzothiazine V, resp. The products III underwent the hydrolytic C2-C3 bond cleavage of the thiazine nucleus to give the α -ketosulfides 2-R1CONHC6H4SCHR2COR. Such a hydrolytic process also explains the formation of IV (R3 = 2-AcNHC6H4S). V is formed through a rearrangement involving the 1,3-sulfur shift of the preformed 1,4-benzothiazine III (R = Ph, R1 = R2 = Me).

IT **124530-81-0P 124530-82-1P**

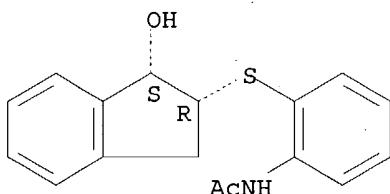
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and basic hydrolysis of)

RN 124530-81-0 CAPLUS

CN Acetamide, N-[2-[(2,3-dihydro-1-hydroxy-1H-inden-2-yl)thiolphenyl]-, cis- (9CI) (CA INDEX NAME)

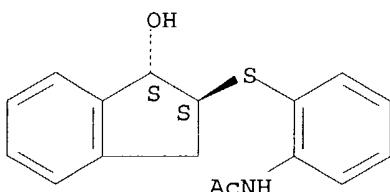
Relative stereochemistry.



RN 124530-82-1 CAPLUS

CN Acetamide, N-[2-[(2,3-dihydro-1-hydroxy-1H-inden-2-yl)thiolphenyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



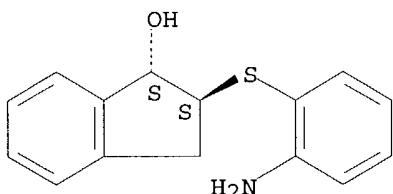
IT 100461-51-6P 124530-84-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 100461-51-6 CAPLUS

CN 1H-Inden-1-ol, 2-[(2-aminophenyl)thio]-2,3-dihydro-, trans- (9CI) (CA
INDEX NAME)

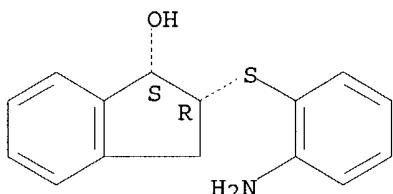
Relative stereochemistry.



RN 124530-84-3 CAPLUS

CN 1H-Inden-1-ol, 2-[(2-aminophenyl)thio]-2,3-dihydro-, cis- (9CI) (CA INDEX
NAME)

Relative stereochemistry.



=> s C16 H16 O2 S/mf and l11

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L17 798 L16

L18 5 L17 AND L11

=> d ibib abs hitstr 3

L18 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:475774 CAPLUS

DOCUMENT NUMBER: 57:75774

ORIGINAL REFERENCE NO.: 57:15030e-i

TITLE: Hydroperoxides and sulfoxides

INVENTOR(S): Oswald, Alexis A.; Rupar, Charles B.; Greenwood,
Sydney H.J.

PATENT ASSIGNEE(S): Esso Research and Engineering Co.

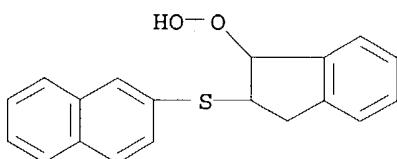
SOURCE: 8 pp.

DOCUMENT TYPE: Patent

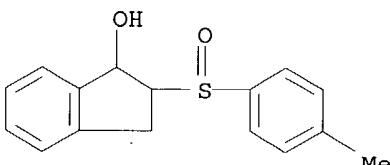
LANGUAGE: Unavailable

PATENT INFORMATION:

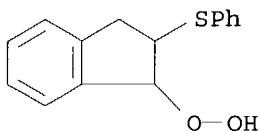
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3043824		19620710	US	19590928
AB	Co-oxidation of RSH with olefins or diolefins in the presence of O at 0° produced new sulfoxides and hydroperoxides. Ultraviolet light and hydroperoxides were found to be effective catalysts for the oxidation. Thus, 20.2 g. n-C ₁₂ H ₂₅ SH and 10.4 g. styrene were dissolved in 150 cc. n-C ₇ H ₁₆ in 500 cc. quartz bottle and irradiated with ultraviolet light (or hydroperoxides added). Air was passed through the solution via sintered glass and filtered after 0.5 hr. to give 18.7% 2-phenyl-2-hydroperoxyethyl n-dodecyl sulfide. Similarly prepared were 1-hydroperoxy-4-phenylthio-2-butene, 1-hydroperoxy-4-(2-naphthylthio)-2-pentene, 2-hydroperoxy-4-(2-naphthylthio)-2cyclopentene, and 4,7-methylene-5-(2-naphthylthio)-6-hydroperoxy-4,5,6,7,8,9-hexahydroindene. The filtrate was treated with air 6 hrs. and filtered to give 9 g. 2-phenyl-2hydroxyethyl n-dodecyl sulfoxide (I), m. 107-9° (benzene-nheptane). The filtrate gave a mixture of isomeric I, m. 66-9°. Similarly prepared were the following sulfoxides, where R ₁ = C ₁₆ H ₃₃ CH(OH)CH ₂ , R ₂ = p-MeC ₆ H ₄ , R ₃ = naphthyl, R ₄ = p-ClC ₆ H ₄ , R ₅ = PhCH(OH)CH ₂ , R ₆ = PhCMe(OH)CH ₂ , R ₇ = C ₁₂ H ₂₅ , and R ₈ = 2-(1-hydroxyindanyl): PhSOCH ₂ CH(OH)C ₁₀ H ₂₁ , m. 67-8°; PhSOR ₁ , m. 51-2°; R ₂ SOR ₁ , m. 60-2°; R ₃ SOR ₁ , m. 88-90°; R ₄ SOR ₁ , m. 65-6.5°; R ₅ SOPh, m. 123-30°; R ₅ SOR ₃ , m. 145-7°; R ₅ SOR ₄ , m. 156.5-8.5°; R ₆ SOR ₃ , m. 114-18°; R ₆ SOR ₇ , m. 47.5-8.5°; R ₈ SOPh, m. 158-9° (decomposition); R ₈ SOR ₂ , 166-7.5° (decomposition); R ₈ SOR ₄ m. 144-6°; R ₈ SOR ₃ , m. 149-50°; and R ₈ SOR ₇ , m. 107-9°. The hydroxy sulfoxide products of dicyclopentadiene-RSH co-oxidns. were useful as petroleum additives, antistatic agents, and pesticides. The OH group may be esterified with H ₂ SO ₄ and converted to detergents. The hydroperoxides are useful as radical polymerization promoters and can be alkylated to give surfactive agents. Co-oxidation can be utilized to remove dienes from steam-cracked naphtha and for removal of RSH from petroleum.			
IT	970-61-6, Hydroperoxide, 2-(2-naphthylthio)-1-indanyl 93434-18-5, 1-Indanol, 2-(p-tolylsulfinyl)- 93898-97-6, Hydroperoxide, 2-(phenylthio)-1-indanyl (preparation of)			
RN	970-61-6 CAPLUS			
CN	Hydroperoxide, 2-(2-naphthylthio)-1-indanyl (6CI, 7CI, 8CI) (CA INDEX NAME)			



RN 93434-18-5 CAPLUS
CN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



RN 93898-97-6 CAPLUS
CN Hydroperoxide, 2-(phenylthio)-1-indanyl (6CI, 7CI) (CA INDEX NAME)



=> d ibib abs hitstr 4-5

L18 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:73337 CAPLUS

DOCUMENT NUMBER: 56:73337

ORIGINAL REFERENCE NO.: 56:14179h-i,14180a-i,14181a-b

TITLE: Organic sulfur compounds. VI. The effect of alkylamines on the course of the cooxidation of mercaptans and indene

AUTHOR(S): Oswald, Alexis A.; Noel, Fernand; Fisk, George

CORPORATE SOURCE: Imp. Oil Co., Sarnia, Can.

SOURCE: Journal of Organic Chemistry (1961), 26, 3974-80

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB In the presence of alkylamines, mercaptans, and indene (I) were cooxidized by mol. O with a chain mechanism to form substituted 2-mercpto-1-indanols, disulfides, and H₂O, instead of substituted 2-mercpto-1-indanyl hydroperoxides. The initiation reaction forming the mercapto radicals could take place between alkylammonium thiolates and O. The change of the reaction products was due to the catalysis by the amines of the oxidation of mercaptans by substituted 2-mercpto-1-indanyl hydroperoxides. It was proposed that this catalytic action was important in the stabilization of some hydrocarbon fuels by alkylamines. In the cooxidn. expts., the O or air was introduced through a sintered glass inductor, mixture stirred, and the pressure kept slightly above atmospheric. The reactions were followed by determining the decrease of the thiol concentration by potentiometric titration of

samples with AgNO₃. 2-(2-Naphthylthio)-1-indanyl hydroperoxide (II) (14.2 g.) in 2.5 l. PhMe, 6.6 g. benzenethiol (IIa), and 7.6 g. 1,1,3,3-tetramethylbutylamine (III) left 0.5 hrs., the solution evaporated in vacuo, at first 2-(2-naphthylsulfinyl)-1-indanol removed, then the solvent evaporated, and from the residue III and diphenyl disulfide removed by leaching with 2 60-ml. portions of heptane, and the product crystallized gave 5.2 g. 2-(2-naphthylthio)-1-indanol (IIIa), m. 141-3° (PhMe). IIa (13.2 g.) and 7.7 g. III in 250 ml. C₆H₆ treated with 19.4 g. 79% 2-phenylthio-1-indanyl hydroperoxide, the mixture stirred another hr. and evaporated, and the residue crystallized gave 5 g. 2-phenylthio-1-indanol (IIIb), m. 103-4° (heptane). A yield of 4.2 g. (PhS)₂ was also obtained in this experiment II (6.3 g.) in 25 ml. Et₂O added slowly to 1.1 g. triethylenediamine in 10 ml. Et₂O (an exothermic reaction occurred) and the solid collected gave 6.7 g. triethylenediammonium 2-(2-naphthylthio)-1-indanyl peroxide (IV), m. 89-90°. The synthesis of IV was also accomplished in PhMe. IIa (1.1 g.) in 80 ml. PhMe treated with 1.8 g. IV (slowly), the mixture left 0.5 hr. and filtered, and the solid recrystd. gave 1.2 g. IIIa. 2-Naphthalenethiol (6.4 g.) in 50 ml. PhMe treated 0.5 hr. at room temperature with 7.3 g. IV gave 8.8 g. addition product (V) of 2-(2-naphthylthio)-1-indanol and di-2-naphthyl disulfide, m. 126-7°

(PhMe). IIIa (1.46 g.) and 1.6 g. di-2-naphthyl disulfide in 25 ml. PhMe heated, cooled to room temperature, and the crystals collected gave 2.5 g. v. A C₆H₆ solution (333 ml.) of 0.34 mole aromatic thiol, 0.11 mole I, and 0.01 mole of an alkylamine was oxygenated 6 hrs. at 22-8°. When benzenethiol and 2-naphthalenethiol were cooxidized with I in the presence of III, a yellow color developed. With 4-butylbenzenethiol, the mixture became dark yellow; with 4-toluenethiol and 4-chlorobenzenethiol, it became red and black, resp. When benzenethiol and I were cooxidized in the presence of mono-, di-, and tripropylamines, the formation of purple, green, and yellow colors were observed. After oxygenation, the C₆H₆ layer was decanted, the unchanged thiol removed from the C₆H₆ solution by washing with 5% KOH solution, the solvent distilled, and the residue fractionated to give 2-arylthio-1-indanols. The diaryl disulfides were too soluble in heptane and therefore were crystallized from MeOH. In the case of the 2-naphthalenethiol-I cooxidn., the reactant concns. were reduced to one-third, and C₆H₆ used as solvent of recrystn. because of the solubility of the addition compound of IIIa and di-2-naphthyl disulfide. The cooxidn. of IIa and I in the presence of III was also carried out on a 5 times larger scale in PhMe. After 6 hrs. of oxygenation, 58% of the thiol was oxidized and 4.4 g. of H₂O separated. By the extraction of the reaction mixture with 5%

HCl

and the concentration of the extract, 7 g. III.HCl was isolated. Workup of the PhMe

solution gave 20.5 g. IIIb. A heptane solution (333 ml.) of 73.3 g. dodecanethiol, 22.9 g. I, and 4.2 g. III was oxygenated at 24-6° and the product, m. 69-72°, isolated. In addition to the above, the following substituted 2-mercaptop-1-indanols were prepared (substituent, m.p., and % yield given): 4-tolyl, 95.5-6.5°, 64; 4-butylphenyl, 104-5°, 39; 4-chlorophenyl, 113.5-14.5°, 35. 2-Arylthio-1-indanol (0.01 mole) in AcOH was treated slowly at 50° with 1.1 g. 33% H₂O₂, the mixture kept 0.5 hr. at 60°, the resulting 2-arylsulfinyl-1-indanol precipitated by addition of H₂O, the solid collected,

and

recrystd. from alc. Most of the oxidation products were identified with one isomer of the substituted 2-sulfinyl-1-indanols from the cooxidn. of I with the corresponding thiol in the absence of amine as shown (thiol starting material, m.p. of the 2-sulfinyl-1-indanol obtained by H₂O₂ oxidation given): benzene, 147-8.5° (decomposition); toluene, 144-5.5° (decomposition); 4-chlorobenzene, 146.5-8.0° (decomposition); 2-naphthalene, 134.5-6.0°; dodecane, 80-1°. An AcOH solution of 0.01 mole of 2-arylthio-1-indanol was oxidized with 2.3 g. 33% H₂O₂ as described above; the work up of the mixture (after being heated 1 hr. at 80°) yielded the 2-arylsulfonyl-1-indanols given below. The following substituted 2-sulfinyl-and 2-sulfonylindanols were thus obtained (R and x of RSO_x, m.p., and % yield given): 4-butylphenyl, 1, 154-6°, 63; 4-dodecyl, 1, 80-1°, 71; 4-tolyl, 2, 145-6.5°, 72; 4-butylphenyl, 2, 156-8°, 98; 4-chlorophenyl, 2, 151.5-4.0°, 95; dodecyl, 2, 93.5-4.5°, 97. Benzene solns. containing 0.15 mole/l. of benzenethiol and 0.05 mole/l. I were oxygenated in the presence of various concns. of III at room temperature. After 6 hrs. of oxygenation, the following decrease in % mercaptan was observed (amine mole/l., % thiol oxidized given): nil, 41; 0.015, 14; 0.150, 48; 0.300, 47. Primene 81-R was added to heptane solns. containing benzenethiol, I, and 2,5-dimethylpyrrole, the test solns. (300 ml. each) were aerated 6 hrs. at room temperature, and the following observations were made (mole/l.

each

of benzenethiol, I, and 2,5-dimethylpyrrole, mole/l. Primene 81-R, % thiol oxidized, peroxide formed, color of solution, and precipitate in g./100 ml. given):

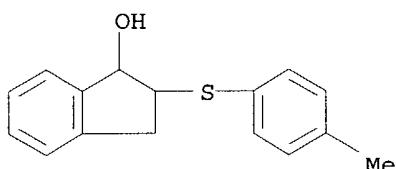
0.30, nil, 68, yes, red, 3.5 (red oil); 0.30, 0.03, 56, no, colorless, 1.3 (colorless crystals); 0.01, nil, 75, yes, red, 0.2 (red solid); 0.01, 0.001, 53, no, colorless, none.

IT 93433-68-2, 1-Indanol, 2-(p-tolylthio)- 93434-18-5,
1-Indanol, 2-(p-tolylsulfinyl)- 93898-88-5, 1-Indanol,

2-(phenylthio)- 94305-32-5, 1-Indanol, 2-(2-naphthylthio)-
94384-90-4, 1-Indanol, 2-[(p-butylphenyl)thio]- **95001-29-9**
, 1-Indanol, 2-(dodecylthio)- **106682-74-0**, Hydroperoxide,
2-(2-naphthylthio)-1-indanyl, compound with 1,4-diazabicyclo[2.2.2]octane
106784-34-3, 1-Indanol, 2-(2-naphthylthio)-, compound with
2-naphthyl disulfide
(preparation of)

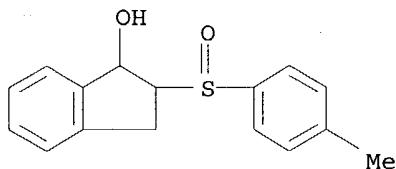
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NAME)



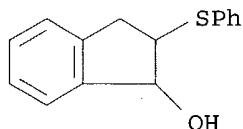
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CN 1H-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



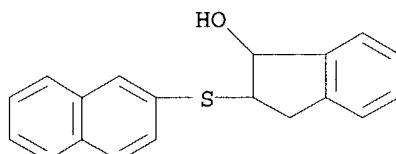
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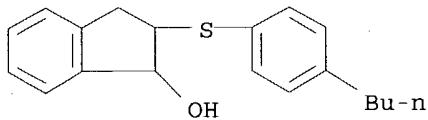
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CN 1-Indanol, 2-(2-naphthylthio)- (7CI) (CA INDEX NAME)

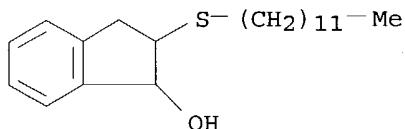


RN 94384-90-4 CAPLUS

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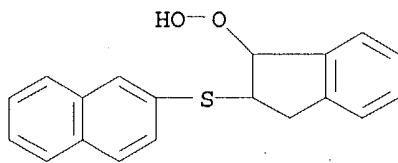
RN 95001-29-9 CAPLUS
CN 1-Indanol, 2-(dodecylthio)- (7CI) (CA INDEX NAME)



RN 106682-74-0 CAPLUS
CN Hydroperoxide, 2-(2-naphthylthio)-1-indanyl, compd. with
1,4-diazabicyclo[2.2.2]octane (7CI) (CA INDEX NAME)

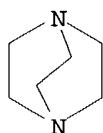
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CRN 970-61-6
CMF C19 H16 02 S



CM 2

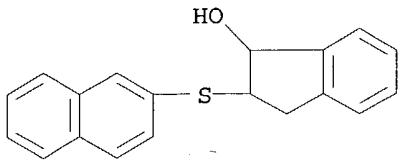
CRN 280-57-9
CMF C6 H12 N2



RN 106784-34-3 CAPLUS
CN 1-Indanol, 2-(2-naphthylthio)-, compd. with 2-naphthyl disulfide (7CI)
(CA INDEX NAME)

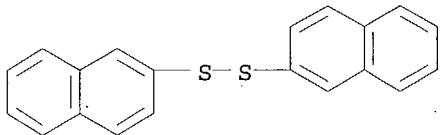
CM 1

CRN 94305-32-5
CMF C19 H16 O S



CM 2

CRN 5586-15-2
CMF C20 H14 S2



L18 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1961:124710 CAPLUS
 DOCUMENT NUMBER: 55:124710
 ORIGINAL REFERENCE NO.: 55:23460b-i, 23461a-c
 TITLE: Organic sulfur compounds. III. Cooxidation of mercaptans with styrenes and indene
 AUTHOR(S): Oswald, Alexis A.
 CORPORATE SOURCE: Imp. Oil Ltd., Sarnia, Can.
 SOURCE: Journal of Organic Chemistry (1961), 26, 842-6
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 54, 21005e. PhSH (I) (0.1 mole) and 0.1 mole PhCH:CH₂ (II) [or PhCMe:CH₂ (III) or indene (IV)] in 310 ml. cold n-C₇H₁₆ bubbled through with air via a sintered glass sparger 6 hrs. at 0° yielded 30, 52, and 33% oily peroxides containing 84, 44, and 67% hydroperoxide, according to both the iodide and FeSO₄ methods. Similar aeration of p-C₁C₆H₄SH and III yielded 64% peroxide containing 58% hydroperoxide. A 4-g. sample of liquid substituted 2-mercptoethyl hydroperoxide kept 3 days at 20° and the solid product recrystd. from PhMe-C₇H₁₆ yielded the corresponding isomeric 2-sulfinylethanol rearrangement products, RSO-CH₂CR'PhOH (V). A typical member of these new hydroperoxides was 1-(2-naphthylthio)-2-phenyl-2-propyl hydroperoxide (VI), m. -10°, peroxide content 85%, obtained by cooxidn. of 2-HSC₁₀H₇ and III. Phys. data were listed for V [R, R', m.p. (uncor.), and infrared OH, SO (2), aromatic and CH₂ absorption peaks given]: Ph, H, 128-9.5°, 2.95, 9.23 (9.55), 10.02, 6.3, 6.9; 2-C₁₀H₇, H, 145-7° (121-6°), 3 (3.05), 9.5 (9.45), 9.9 (9.9), 6.28 (6.28), 6.91 (6.91); C₁₂H₂₅, H, 105-6° (69-70°), 3 (3), 9.3 (9.3), 9.85 (9.85), 6.25 (6.25), 6.9 (6.9); 4-C₁C₆H₄, H, 156.5-8.5° (86-8°), 2.96 (2.96), 9.19 (9.19), 9.94 (9.96), 6.35 (6.35), 6.95 (6.95); 2-C₁₀H₇, Me, 115-18° (94-95.5°), 3.05 (3), 9.4 (9.4), 9.95 (9.78), 6.28 (6.28), 6.85 (6.93); C₁₂H₂₅, Me, 47.5-8.5°, 2.95, 9.4, 10.05, 6.25, 6.85. Similar rearrangements were carried out in 0.3M C₆H₆ (CHCl₃, tetrahydronaphthalene) solns. of hydroperoxides at 43° in 16 hrs. VI (3.1 g.) yielded 27% V (R = 2-C₁₀H₇, R' = H), m. 115-18°, by this method. IV (11.6 g.) and 16 g. 2-C₁₀H₇SH in 100 ml. C₆H₆ and 300 ml. C₇H₁₆ aerated 4 hrs. at 0° yielded 4 g. crystalline 2-(2-naphthylthio)-1-

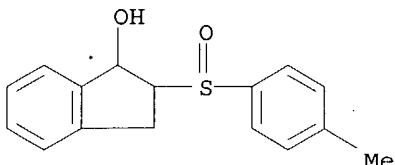
indanyl hydroperoxide (VII), m. 70° (decomposition), containing 98% peroxide. The filtrate aerated 6 hrs. at 0° and 42 hrs. at 20°, filtered, and the cooxidn. product (26 g., containing only 2% peroxide) recrystd. from C₆H₆-C₇H₁₆ gave the 2-(2-naphthylsulfinyl)-2-indanoisomers, C₆H₄.CH(OH).CH(SOR).CH₂ (VIII, R = 2-C₁₀H₇) (IX), m. 157-8°, m. 149-50°, m. 138.5-9.5° (decomposition), m. 125-7.5° (decomposition) (infrared spectrum given for all). VII (9.2 g.) in 100 ml. C₆H₆ kept 16 hrs. at 43° gave a neg. peroxide test and deposited 36.8 g. crystals, m. 138.5-9.5° (C₆H₆), identical with an isomer of IX. VII stored 10 min. in a desiccator at 2 mm. over H₂SO₄ decomposed violently and the reddish product fractionally crystallized from

C₆H₆ gave IX, m. 157-8° and 138.5-9.5°. IV (10.7 g.) and 12.8 g. 4-ClC₆H₄SH in 250 ml. C₆H₆ and 20 ml. PhCl at 0° aerated 4 hrs. and the fresh peroxide solution refluxed 1 hr. in Et₂O with LiAlH₄ yielded 68% 2-(4-chlorophenylthio)-1-indanol (X), m. 110-12°. VII (6.0 g.) in 600 ml. C₆H₆, 150 ml. CHCl₃, and 20 ml. MeOH kept 3 days at 20° with 4.3 g. X gave unchanged X and IX, m. 157-8°, suggesting an intramol. rearrangement. However, the reactions of the hydroperoxide cooxidn. intermediate might involve radical intermediates as was suggested by the polymerization of II by VII. VII (0.3 g.) in 34.6 g. II kept 3 months at 5° gave only 75% recovered II on distillation at 100°/20 mm., whereas II kept alone under the same conditions was distilled with 99% recovery. Aliphatic hydrocarbon (C₇H₁₆, cetane, straight run petroleum distillate, b. 70-200°) (300 ml.) containing 0.1 mole thiol, p-RC₆H₄SH (R = H, Me, 4-ClC₆H₄, and II, III, or IV aerated (or oxygenated) 3 days at 20° to give a liquid phase with peroxide number and mercaptan number less than 5 and 10, resp., the residue on filtration recrystd. from Ph-Me-C₇H₁₆ to give 40-80% mixts. of isomeric substituted 2-sulfinyl ethanols, and the mixts. recrystd. gave (with about 30% yield loss) the isomeric VIII (R and m.p. given) (infrared spectra given): Ph, 158-9°; 148-50°, 132-5°; p-MeC₆H₄, 166-7.5°, 144-4.5°, 128-30°; p-ClC₆H₄, 144-6°; C₁₂H₂₅, 107-9°, 67-8.5°. C₁₂H₂₅SH (20.2 g.) and 0.1 mole II (III, IV) in 300 ml. C₇H₁₆ aerated in a Vycor (95% quartz) flask with ultraviolet irradiation (GE-9T64Y20 lamp, 250 v., 1000 w. at 4.5 cm.) with decrease to less than 10% thiol content, the mixture cooled (solid CO₂-alc. bath), and the product recryst. gave 75% VIII (R = C₁₂H₂₅) isomers. Cooxidn. of C₁₂H₂₅SH with III and IV gave only 10% V (R = C₁₂H₂₅, R' = Me) and 31% VIII (R = C₁₂H₂₅), m. 107-9°. Cetane (300 ml.) containing 0.01 mole/l. 2-C₁₀H₇SH and 0.01 mole II (IV) kept in a 500 ml. open pyrex flask showed rapid peroxidn. followed by a decrease in peroxide content, though the components in cetane showed no peroxidn. After 70 and 23 hrs. the IV-thiol and II-thiol solns. gave some IX, m. 138.5-9.5° (decomposition), and V (R = 2-C₁₀H₇, R' = H), m. 145-7°. Cetane (300 ml.) containing 0.3 mole/l. mercaptans and II or IV kept 2 weeks in accelerated storage tests at 43° and the ppts. recrystd. from C₆H₆-C₇H₁₆ gave the corresponding VIII. Distillation of the mother liquors yielded about 200 mg. 2-indanyl Ph sulfide and 180 mg. 2-indanyl 4-tolyl sulfide, resp. The reported reactions may be important in causing hydrocarbon fuel instability.

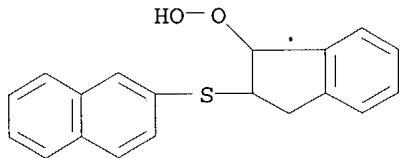
IT 93434-18-5, 1-Indanol, 2-p-tolylsulfinyl-
(isomers)

RN 93434-18-5 CAPLUS

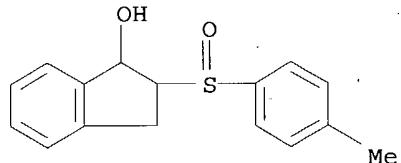
CN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)



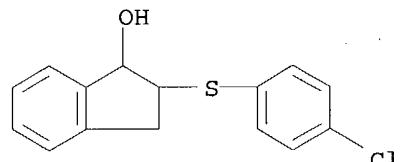
IT 970-61-6, Hydroperoxide, 2-(2-naphthylthio)-1-indanyl
93434-18-5, 1-Indanol, 2-p-tolylsulfinyl- 97636-30-1,
1-Indanol, 2-(p-chlorophenylthio)-
(preparation of)
RN 970-61-6 CAPLUS
CN Hydroperoxide, 2-(2-naphthylthio)-1-indanyl (6CI, 7CI, 8CI) (CA INDEX
NAME)



RN 93434-18-5 CAPLUS
CN 1-Indanol, 2-(p-tolylsulfinyl)- (6CI, 7CI) (CA INDEX NAME)

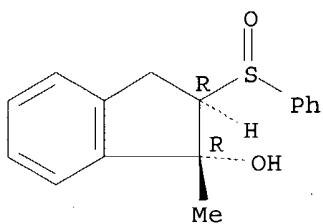


RN 97636-30-1 CAPLUS
CN 1H-Inden-1-ol, 2-[{(4-chlorophenyl)thio]-2,3-dihydro- (9CI) (CA INDEX
NAME)



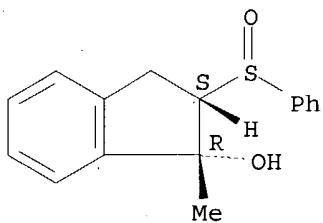
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Relative stereochemistry.

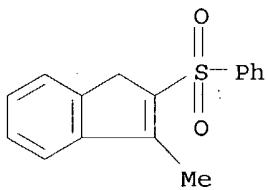


RN 155519-29-2 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfinyl)-,
(1 α ,2 α) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 155519-30-5 CAPLUS
CN 1H-Indene, 3-methyl-2-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



Structure attributes must be viewed using STN Express query preparation.

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100.0% PROCESSED 988 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

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BATCH **COMPLETE**
PROJECTED ITERATIONS: 17875 TO 21645
PROJECTED ANSWERS: 0 TO 0

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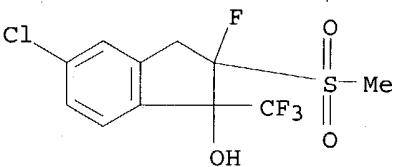
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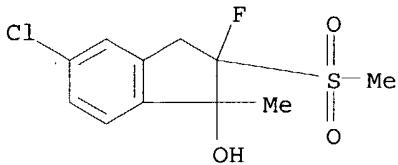
L3 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN
RN 501083-94-9 REGISTRY
CN 1H-Inden-1-ol, 5-chloro-2-fluoro-2,3-dihydro-2-(methylsulfonyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H9 Cl F4 O3 S
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN
RN 501083-93-8 REGISTRY
CN 1H-Inden-1-ol, 5-chloro-2-fluoro-2,3-dihydro-1-methyl-2-(methylsulfonyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H12 Cl F O3 S
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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FULL ESTIMATED COST		ENTRY	SESSION
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FILE COVERS 1907 - 27 Apr 2004 VOL 140 ISS 18
FILE LAST UPDATED: 26 Apr 2004 (20040426/ED)

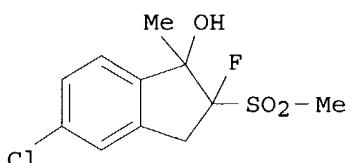
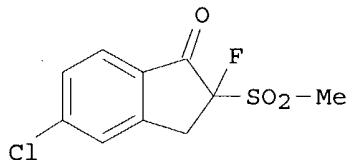
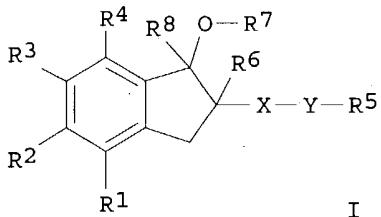
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
L4 2 L3

=> d ibib abs hitstr 1-2

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2003:202615 CAPLUS
 DOCUMENT NUMBER: 138:237904
 TITLE: Preparation of indan-1-ols as appetite depressants
 INVENTOR(S): Jaehne, Gerhard; Krone, Volker; Bickel, Martin;
 Gossel, Matthias
 PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany
 SOURCE: PCT Int. Appl., 45 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020693	A1	20030313	WO 2002-EP9201	20020817
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10142661	A1	20030327	DE 2001-10142661	20010831
US 2003105145	A1	20030605	US 2002-231362	20020830
US 6670401	B2	20031230		
PRIORITY APPLN. INFO.:			DE 2001-10142661 A 20010831	
OTHER SOURCE(S) :			MARPAT 138:237904	
GI				



AB Title compds. I [R1, R2, R3, R4 = H, halo, CN, etc.; X = S, SO, SO2; Y = (CH₂)_p; p = 0-3; R5 = alkyl, cycloalkyl, (CH₂)₁₋₆CO₂H, etc.; R6 = (CH₂)₀₋₆R₉, (CH₂)₀₋₆CO₂H, (CH₂)₀₋₆CONH₂, etc.; R7 = (CH₂)₀₋₄R₁₂, H, alkyl, etc.; R8 = (CH₂)₀₋₄R₁₄, alkyl, cycloalkyl, etc.; R9, R₁₂, R₁₄ = Ph, 1-naphthyl, 2-naphthyl, etc.] and their pharmaceutically acceptable salts were prepared. For example, MeMgBr carbonyl addition to indanone II, e.g., prepared from 2-bromo-5-chloroindan-1-one in 3-steps, provided indanol III. In milk consumption studies with female NMRI mice, indanol III exhibited very good anorectic effects, i.e., 25% decrease in milk consumption versus control.

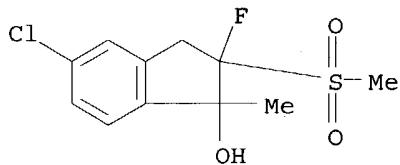
IT 501083-93-8P 501083-94-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

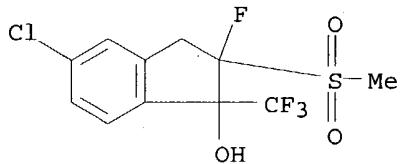
(drug candidate; preparation of indanols as appetite depressants)

RN 501083-93-8 CAPLUS

CN 1H-Inden-1-ol, 5-chloro-2-fluoro-2,3-dihydro-1-methyl-2-(methylsulfonyl)- (9CI) (CA INDEX NAME)



RN 501083-94-9 CAPLUS
 CN 1H-Inden-1-ol, 5-chloro-2-fluoro-2,3-dihydro-2-(methylsulfonyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



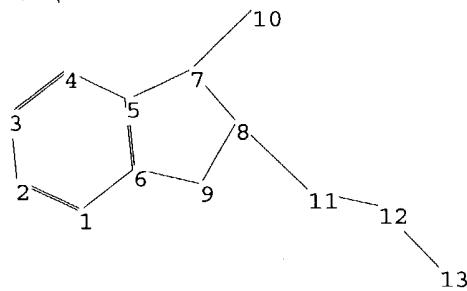
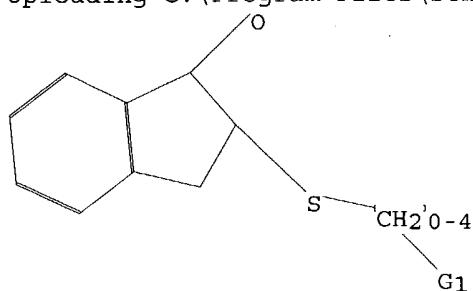
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2003:202458 CAPLUS
 DOCUMENT NUMBER: 138:221359
 TITLE: Preparation of indan-1-ols for producing drugs for the prophylaxis or treatment of obesity
 INVENTOR(S): Jaehne, Gerhard; Krone, Volker; Bickel, Martin;
 Gossel, Matthias
 PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
 SOURCE: PCT Int. Appl., 47 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020255	A1	20030313	WO 2002-EP9200	20020817
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10142659	A1	20030320	DE 2001-10142659	20010831
US 2003130323	A1	20030710	US 2002-230353	20020829
US 6686397	B2	20040203		

PRIORITY APPLN. INFO.: DE 2001-10142659 A 20010831
 OTHER SOURCE(S): MARPAT 138:221359
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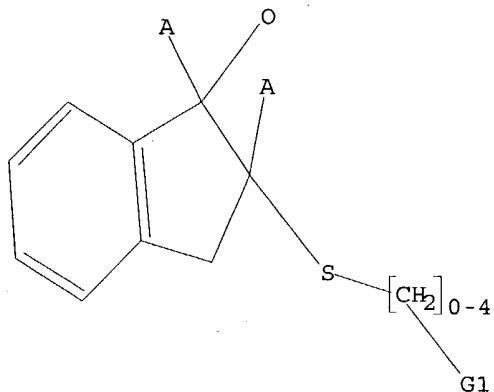
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exact/norm bonds :
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G1:Cy,Ak

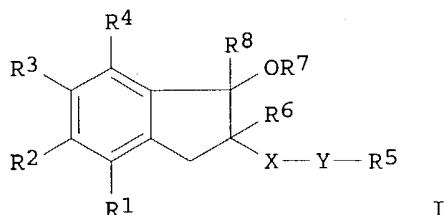
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Match level :
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11:CLASS 12:CLASS 13:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 Cy,Ak



AB Title compds. [I; R1-R4 = H, F, Cl, Br, I, cyano, N3, NO₂, OH, alkoxy, cycloalkoxy, benzyloxy, phenoxy, alkylcarbonyloxy, etc.; or R₂R₃ = OCH₂O; X = S, SO, SO₂; Y = (CH₂)_p; p = 0-3; R₅ = (fluorinated) alkyl, cycloalkyl, etc.; R₆ = (substituted) alkyl, et.; R₇ = H, (substituted) alkyl, cycloalkyl, etc.; R₈ = (substituted) alkyl, cycloalkyl], were prep'd for producing a drug for body weight loss of mammals. Thus, 5-chloro-2-fluoro-2-methanesulfonylindan-1-one (preparation given) in THF was dropwise treated with MeMgBr in Et₂O followed by stirring for 3 h at 50°, further addition of MeMgBr, and stirring for 1h at room temperature to give 5-chloro-2-fluoro-2-methanesulfonyl-1-methylindan-1-ol. The latter at 30 mg/kg i.p. was applied in female NMRI mice and gave 25% reduction of milk consumption of the treated mice.

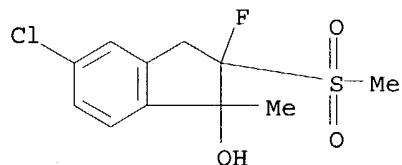
IT 501083-93-8P 501083-94-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indanols for producing drugs for the prophylaxis or treatment of obesity)

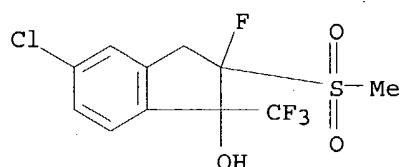
RN 501083-93-8 CAPLUS

CN 1H-Inden-1-ol, 5-chloro-2-fluoro-2,3-dihydro-1-methyl-2-(methylsulfonyl)- (9CI) (CA INDEX NAME)



RN 501083-94-9 CAPLUS

CN 1H-Inden-1-ol, 5-chloro-2-fluoro-2,3-dihydro-2-(methylsulfonyl)-1-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

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THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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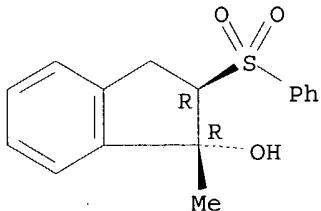
=> s 13

L4 1 L3

=> d ibib abs hitstr 1-3

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STM
ACCESSION NUMBER: 1994:409577 CAPLUS
DOCUMENT NUMBER: 121:9577
TITLE: Reactions of η^2 - (2-acylaryl-C,O)tetracarbonylmanganese(I) complexes with some vinyl sulfur compounds
AUTHOR(S): Cambie, Richard C.; Rutledge, Peter S.; Welch, David R.; Woodgate, Paul D.
CORPORATE SOURCE: Department of Chemistry, University of Auckland, Private Bag 92019, Auckland, N. Z.
SOURCE: Journal of Organometallic Chemistry (1994), 467(2), 237-44
CODEN: JORCAI; ISSN: 0022-328X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:9577
AB The thermally promoted reactions of some Ph and diterpenoid η^2 - (2-acylaryl-C,O)tetracarbonylmanganese(I) complexes with Ph vinyl sulfone, Me vinyl sulfone, or Ph vinyl sulfoxide, have been investigated. The major products from the diterpenoid complexes arises from insertion followed by reductive demetalation; cyclopenta-annulation, when it occurs, is a minor process. Liberation of the metal-free adducts from their Mn-containing precursors requires treatment with either acid or photolysis-oxidation
IT 155519-26-9P 155519-27-0P 155519-28-1P
155519-29-2P 155519-30-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 155519-26-9 CAPLUS
CN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfonyl)-, trans- (9CI) (CA INDEX NAME)

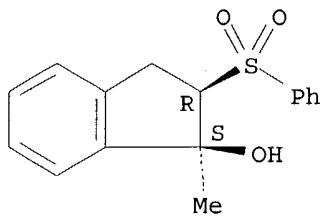
Relative stereochemistry.



RN 155519-27-0 CAPLUS

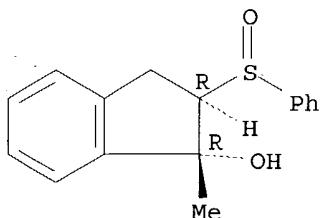
CN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfonyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



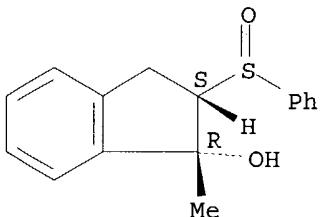
RN 155519-28-1 CAPLUS
 CN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfinyl)-,
 (1 α ,2 β) - (9CI) (CA INDEX NAME)

Relative stereochemistry.

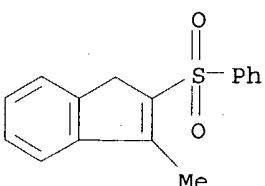


RN 155519-29-2 CAPLUS
 CN 1H-Inden-1-ol, 2,3-dihydro-1-methyl-2-(phenylsulfinyl)-,
 (1 α ,2 α) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 155519-30-5 CAPLUS
 CN 1H-Indene, 3-methyl-2-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



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